From local to nonlocal Fermi liquid in doped antiferromagnets

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The variation of single-particle spectral functions with doping is studied numerically within the t-J model. It is shown that corresponding self energies change from local ones at the intermediate doping to strongly nonlocal ones for a weakly doped antiferromagnet. The nonlocality shows up most clearly in the pseudogap emerging in the density of states, due to the onset of short-range antiferromagnetic correlations.

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The understanding of electron spectral properties in the normal-state of cuprate superconductors remains one of the hardest challenges for theoreticians. The single-electron spectral function is directly related to angle-resolved photoemission spectroscopy (ARPES) experiments, which made impressive progress in the last decade [1], in particular in the studies of the development as function of the hole-doping [2,3] with respect to the reference antiferromagnetic (AFM) material. ARPES on optimally doped materials reveals electronic excitations with a large Fermi surface (FS) with the volume consistent with the normal Fermi liquid (FL) picture. The shape of spectral functions is more controversial [1], being possibly closer to the concept of a marginal FL [4] than that of a usual Landau FL. Recently most interesting ARPES results have been obtained for underdoped Bi-SrCaCuO compounds [2,3], where a leading-edge shift at $T > T_c$ indicates a feature consistent with d-wave superconductivity persisting in the normal state. A pseudogap (although much larger) is observed also in the integrated photoemission of LaSrCuO cuprates [5]. These phenomena are closely related to relevant energy scales in doped AFM. In underdoped cuprates experiments confirm that besides T_c a crossover $T^* > T_c$ [6], pronounced in the spin susceptibility χ_0 and in transport quantities $\rho(T)$, $R_h(T)$, and a lower one T_{sg}, most clearly seen in the NMR relaxation.

Most theoretical calculations of spectral functions $A(\mathbf{k},\omega)$ in doped 2D AFM rely on numerical approaches [7]. The exact diagonalization results for the t-J model [8] and the quantum Monte Carlo results for the Hubbard model [9] provide the evidence that prototype models indeed yield a large FS at the intermediate doping with the quasiparticle (QP) dispersion close to the experiment and a 2D tight-binding band. A recent application of the finite-temperature Lanczos method [10,11] in the same regime allows for additional conclusions for spectral functions [12]: a) $A(\mathbf{k},\omega)$ is strongly asymmetric with respect to the FS, with underdamped QP for $k > k_F$ and essentially overdamped QP for $k < k_F$, c) the self-energy follows the marginal FL form $\mathrm{Im}\,\Sigma \sim \gamma(|\omega| + \xi T)$. The regime of low but finite doping is even harder to examine. Among the few studies of $A(\mathbf{k},\omega)$ only the quantum Monte Carlo results [13] seem to indicate the existence of a pseudogap.

In the present Letter we point out two new and unexpected features of the t-J model as a function of doping. The first is that at intermediate doping $A(\mathbf{k},\omega)$ is well accounted for by the assumption of the local FL [14], where the self-energy is like that recently invoked in the context of infinite-dimensional models [15]. The second new feature is in the underdoped regime. Reducing the doping towards an undoped AFM the nonlocality becomes essential, leading to a pseudogap in the single-electron density of states (DOS).

We study the planar t-J model as the prototype model for strongly correlated electrons in a doped AFM,

$$H = -t \sum_{\langle ij\rangle s} (\tilde{c}^\dagger_{js}\tilde{c}_{is} + \mathrm{H.c.}) + J \sum_{\langle ij\rangle} (\mathbf{S}_i \cdot \mathbf{S}_j - \frac{1}{4} n_i n_j) \quad (1)$$

with projected operators $\tilde{c}_{is} = c_{is}(1 - n_{i,-s})$ preventing the double occupation of sites. The Green's function can be defined in the usual way $G(\mathbf{k},\omega) = \langle\langle \tilde{c}_{\mathbf{k}s}; \tilde{c}^\dagger_{\mathbf{k}s}\rangle\rangle_{\omega+\mu}$ where μ is the chemical potential.

It should be stressed that $A(\mathbf{k},\omega) = -(1/\pi)\mathrm{Im}G(\mathbf{k},\omega)$ is not normalized to unity [8,12], since $\langle\{\tilde{c}_{\mathbf{k}s}, \tilde{c}^\dagger_{\mathbf{k}s}\}_+\rangle = (1 + c_h)/2 = \alpha < 1$. This introduces some ambiguity in the definition of Σ. We choose here the one which guarantees the analytical behavior, $\Sigma(\mathbf{k}, \omega \to \pm\infty) = 0$ [16] (in contrast to the definition in Ref. [12]),

$$G(\mathbf{k},\omega) = \frac{\alpha}{\omega + \mu - \zeta_{\mathbf{k}} - \Sigma(\mathbf{k},\omega)}, \quad (2)$$

The 'free' propagation term $\zeta_{\mathbf{k}}$ is nontrivial, since the hopping term in Eq.(1) involves projected operators. It is given by [16]

$$\zeta_{\mathbf{k}} = \frac{1}{\alpha}\langle\{[\tilde{c}_{\mathbf{k}s}, H], \tilde{c}^\dagger_{\mathbf{k}s}\}_+\rangle = \bar{\epsilon} + \epsilon_{\mathbf{k}},$$
$$\epsilon_{\mathbf{k}} = \eta t \gamma_{\mathbf{k}}, \qquad \eta = \alpha + \frac{1}{\alpha}\langle S^z_i S^z_j\rangle, \quad (3)$$

where $\gamma_{\mathbf{k}} = \sum_{j\ n.n.0} \exp(i\mathbf{k}\cdot\mathbf{r}_j)$. Note that η represents the overall renormalization of the spectral dispersion, not just of the QP part. Since n.n. correlation $\langle S_i^z S_j^z\rangle$ decreases with doping one can conclude from Eq.(3) that at the intermediate doping $\eta \sim \alpha \lesssim 0.5$ while in a weakly doped AFM $\eta \sim 0.27$.

We focus on the doping dependence of the $A(\mathbf{k},\omega)$, the corresponding $\Sigma(\mathbf{k},\omega)$ and the DOS, defined by $\mathcal{N}(\epsilon) = (2/N)\sum_{\mathbf{k}} A(\mathbf{k},\epsilon-\mu)$. Calculations are performed at $T>0$ and on small square lattices with $N=16,18$ and 20 sites using the finite-T Lanczos method [10,11]. We fix $J=0.3\ t$ to be representative of strongly correlated systems and of cuprates in particular, where $t\sim 0.4$ eV. It is important to realize that the results are meaningful for $T>T_{fs}$. T_{fs} is the temperature where finite-size effects start to dominate. In available systems $T_{fs}\gtrsim 0.1\ t$ at the intermediate doping $0.1<c_h<0.25$ while it is increasing towards undoped AFM, e.g. $T_{fs}\gtrsim 0.2\ t$ for $c_h\to 0$ [11].

Results for $A(\mathbf{k},\omega)$ at intermediate doping have been partly presented and discussed previously [12]. We point out here a novel aspect of the results, i.e. a nearly $\mathbf{k}$ independent self-energy, $\Sigma(\mathbf{k},\omega)\sim\Sigma_L(\omega)$. We show in Fig. 1a Re$\Sigma$ obtained for $c_h=3/16$, which reveal a weak variation with $\mathbf{k}$. This behavior is characterstic of a local FL [14,15]. This is in a sharp contrast to a strong $\mathbf{k}$ dependence of the self-energy in the underdoped case in Fig. 1b. One of the essential consequences of the local FL is that the DOS at the FS $\mathcal{N}(\mu)$ is independent of the self-energy, being (usually) equal to that of noninteracting fermions. Note, however, that in the t-J model also the 'free' electron dispersion $\zeta_{\mathbf{k}}$ is renormalized, as follows from Eq.(3). Nevertheless the DOS for $c_h=3/16, 4/16$ [12] reveal a smooth variation $\mathcal{N}(\epsilon\sim\mu)\propto 1/\alpha$.

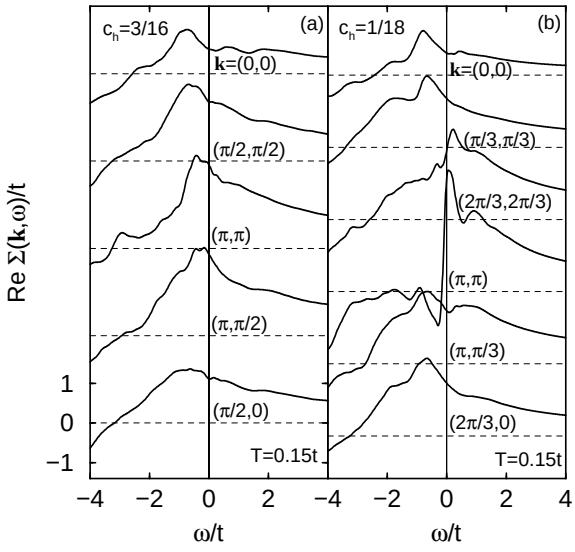

FIG. 1. Self energies Re$\Sigma(\mathbf{k},\omega)$ for the doping: a) $c_h=3/16$, and b) $c_h=1/18$, both for $T=0.15\ t$.

The local FL character is lost entering the underdoped regime. We show in Fig. 2 $A(\mathbf{k},\omega)$ for the lowest concentrations $c_h=0$ and $c_h\sim 0.06$, combining systems with $N=16$ and $N=18$ sites, for the lowest $T\sim T_{fs}$. Rather well understood limit (at least for $T\to 0$) is $c_h=0$, where one is studying a hole in an spin background with the long range AFM order. Note that $T>0$ and $c_h\to 0$ requires $\mu\to-\infty$ hence it is meaningful to present $A(\mathbf{k},\epsilon)$. Consistent with analytical approximations [17] the spectral function shows a coherent QP peak with a dispersion on the energy scale determined by J (bandwidth $W\sim 2J$), with the maximum at $\mathbf{k}^*=(\pi/2,\pi/2)$ with $\epsilon_0\sim 2t$. In addition to a QP feature there is a broad incoherent background for $\epsilon\ll\epsilon_0$. The latter has still some structure, which must be related to the AFM order, since it disappears for $T>J$. For $c_h=0$ the dispersion corresponds to a double AFM unit cell hence the local FL cannot apply.

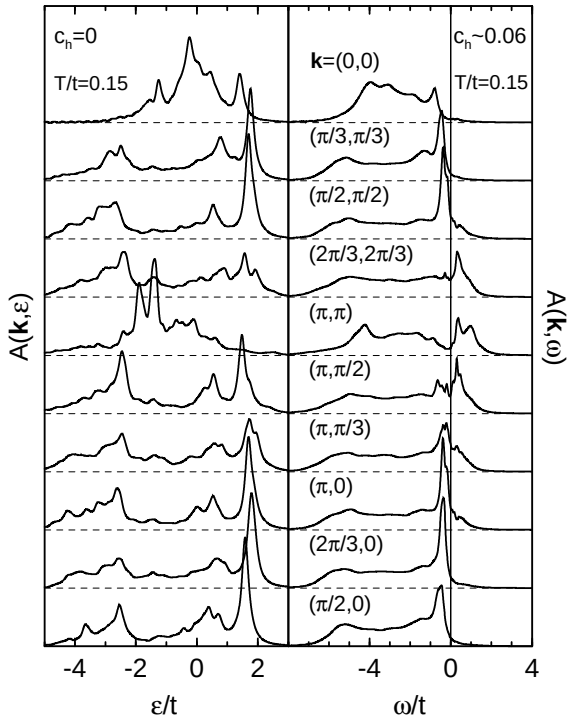

FIG. 2. Spectral functions for the undoped AFM (left), and for system with finite doping $c_h=1/N$, where results for $N=16,18$ are combined for fixed $T=0.15\ t$.

More challenging are results for $c_h\sim 0.06$, also shown in Fig. 2. $A(\mathbf{k},\omega)$ in this regime merge some properties of the undoped AFM and of the intermediate doping. As expected for $c_h>0$ there is besides a hole ($\omega<0$) part also an electron part with $\omega>0$, its integrated intensity increasing as $2c_h$. It is evident that the electron part is significant only for $k>k_F$, i.e. for $\mathbf{k}$ outside the FS which seems to be close to the square AFM Brillouin zone. Another fact is that in $A(k>k_F,\omega)$ with a QP peak at $\omega>0$ there is also a shadow feature for $\omega<0$,

most pronounced for $\mathbf{k} = (\pi, \pi/3), (\pi, \pi/2)$ as well as for $\mathbf{k} = \mathbf{Q} = (\pi, \pi)$. In fact the hole part shows a dispersion very analogous to the one at $c_h = 0$, since the dispersion seems to fold back for $k > k_F$. This is best seen near the X point $\mathbf{k} = (\pi, 0)$ where the hole dispersion does not seem to reach $\omega = 0$, hence an apparent gap between the hole and the electron QP persists. The folding effect is hardly visible along the diagonal Γ-M, i.e. for $\mathbf{k} = (x, x)$, where the QP peak disperses through the FS in a more normal way.

Gap features appear best visible in the DOS which as a local quantity is less affected by finite size effects. In Fig. 3 we show $\mathcal{N}(\epsilon)$ for three lowest dopings $c_h = 0/20, 1/20, 2/18$ and different $T \leq J$. For $c_h > 0$ the vertical line denotes the chemical potential $\mu(T = 0.1\ t)$. While at larger doping the DOS does not show any sign of a gap at the the Fermi energy $\epsilon \sim \mu$ (at least not for $T \gtrsim T_{fs}$) [12], it is evident from Fig. 3 that the pseudogap starts to emerge for $c_h = 2/18$ and is well pronounced for $c_h = 1/20$.

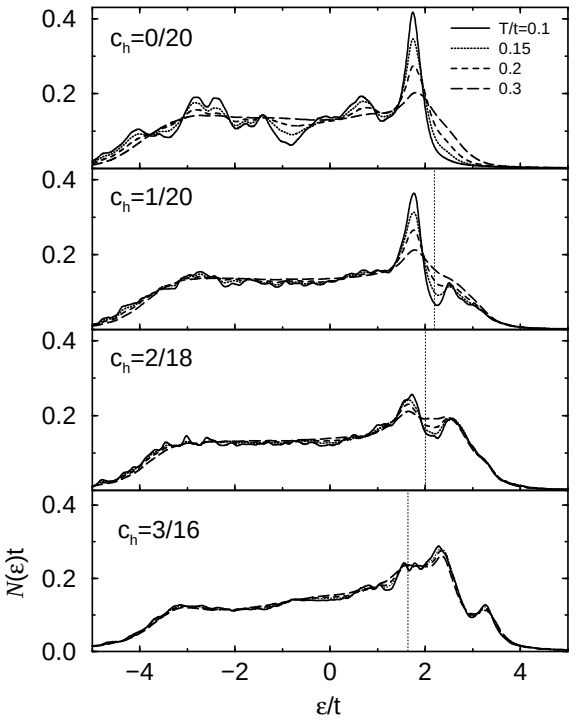

FIG. 3. Density of states $\mathcal{N}(\varepsilon)$ for systems with various doping $c_h = 0/18, 1/18, 2/18$ and different T. The thin vertical lines denote the chemical potemtial $\mu(T = 0.1\ t)$.

The temperature dependence of the DOS is very instructive. It is plausible that for $c_h = 0$ the QP (spin-polaron) propagation [17] becomes incoherent for $T > J$ due to lost AFM short range order, hence a QP peak in $\mathcal{N}(\epsilon)$ broadens. It is interesting to note that at $T \sim J$ some sharper resonances as well disappear in the 'incoherent' part $\epsilon \ll \epsilon_0$. These resonant features at $c_h = 0$ and $T \to 0$ can be interpreted as real excited resonance states of the spin-polaron [17]. The latter are smeared out due to the spin disorder at $T > J$ or due to the presence of other holes as concluded from Fig. 3 for $c_h > 0$ where no such resonances are visible.

A novel feature is the pseudogap at $\epsilon \sim \mu$. The latter is not a finite-size effect since very similar results are obtained e.g. for systems 1/16 and 1/18 [12]. The structure disappears for $T > J$, hence it must be related to the onset of the short-range AFM order. Also its energy span $\Delta\epsilon < t$ seems to be determined rather by J. The pseudogap is inconsistent with the concept of the local FL, since the latter assumption would lead to an enhanced $\mathcal{N}(\mu)$ for $c_h \to 0$ due to reduced η, Eq.(3). Hence the pseudogap can be accounted only by a pronounced nonlocality, i.e. $\mathbf{k}$ dependence of $\Sigma(\mathbf{k} \sim \mathbf{k}_F, \omega \sim 0)$.

The underlying scenario is that the system remains a FL with a well defined FS and a conserved (large) FS volume. This requires at least $\mathrm{Im}\Sigma(\mathbf{k}_F, 0) \to 0$ for $T \to 0$ whereby the FS is determined by $\zeta_{\mathbf{k}_F} = \mu - \mathrm{Re}\Sigma(\mathbf{k}_F, 0)$. Our numerical results for a weakly doped AFM seem to be qualitatively consistent with these assumptions. Note that alternative scenarios have been proposed for the regime of weak doping e.g. invoking a small hole-pocket FS [18]. The FL assumption leads to the usual form for the DOS,

$$\mathcal{N}(\mu) = \frac{2\alpha}{N} \sum_{\mathbf{k}} \delta(\mu - \zeta_{\mathbf{k}} - \mathrm{Re}\Sigma(\mathbf{k}, 0)). \qquad (4)$$

The pseudogap thus requires a large $|d\mathrm{Re}\,\Sigma(\mathbf{k}, 0)/d\mathbf{k}|$ at $\mathbf{k} = \mathbf{k}_F$. In Fig. 1b we show $\mathrm{Re}\,\Sigma(\mathbf{k}, \omega)$ at $c_h = 1/18$ and fixed $T = 0.15\ t$. First we realize that $\mathrm{Re}\Sigma(\mathbf{k}, 0) = \mu - \zeta_{\mathbf{k}}$ locates the presumed FS again close to the AFM zone boundary. The differences with respect to intermediate doping [12] are easily observed. While for $\mathbf{k}$ inside the FS the self-energy is quite similar to the local FL, there is an increasing deviation from the latter for $k > k_F$. In particular this shows up as an oscillation in $\mathrm{Re}\Sigma(\mathbf{k}, \omega)$ most pronounced for $\mathbf{k} = \mathbf{Q}$. The effect is so strong that it leads for most $k > k_F$ to a double solution for a QP peak, i.e. $E_{\mathbf{k}} = \zeta_{\mathbf{k}} + \mathrm{Re}\Sigma(\mathbf{k}, E_{\vec{k}}) - \mu$, explaining the shadow features and folded spectra in Fig. 2 for most $\mathbf{k}$ outside the FS.

The double solutions for $E_{\mathbf{k}}$ are analogous to those appearing within the spin-bag theory [19] taking into account the AFM short-range order. The essential difference is however an evident asymmetry since no such effect appears for $\mathbf{k}$ inside the FS. To simulate the observed corrections to Σ_L due to AFM correlations can be designed. For a long-range AFM order one could expect the form

$$\Sigma(\mathbf{k}, \omega) \sim \Sigma_L(\omega) + a(\mathbf{k}) G(\mathbf{k} + \mathbf{Q}, \omega). \qquad (5)$$

The expression (5) naturally leads to oscillations in $\Sigma(\mathbf{k}, \omega)$ and possible double QP solutions, in particular near the half-filling where the FS is close to the nesting AFM zone boundary. In order to account for the

pronounced asymmetry with respect to FS one has to assume an essential dependence of $a(\mathbf{k})$, i.e. $a(k \ll k_F) \sim 0$ and its strong increase near k_F.

It is however still feasible that in a weakly doped AFM the emerging pseudogap coexists with a well defined large FS. AFM correlations open a pseudogap between the hole-like and electron-like QP resonances coexisting for $\mathbf{k} \sim \mathbf{k}_F$, visible in particular near the X point in Fig. 2. Here it seems that the QP dispersion does not traverse the FS. But the assumption $\mathrm{Im}\Sigma(\mathbf{k}, 0) = 0$ at $T \to 0$ leads to another QP crossing the FS. The latter peak must be of a small QP weight $\tilde{Z} = Z_{\mathbf{k}_F}$. This could be consistent with the inequality $\tilde{Z} < 2c_h$ [12] derived on the assumption of the monotonous fall-off of $\bar{n}_{\mathbf{k}}$. Such a QP excitation would be hard to observe in numerical calculations as well as in experiments since it can be easily overdamped either by $T > 0$ or other effects.

Let us turn to the discussion of the relation of our results to photoemission experiments on cuprates. The latter capture mostly the hole-part $\omega < 0$. For the intermediate doping our $A(\mathbf{k}, \omega)$ are qualitatively consistent with ARPES measurements [1], as discussed in Ref. [12]. ARPES on underdoped BiSrCaCuO compounds [2] shows an opening of a pseudogap near the X point where the FS seems to disappear. On the other hand the QP peak disperses through the FS along the Γ-M direction, rather like in a normal FL. Both facts are well consistent with results in Fig. 2. Recently the DOS has been measured via the integrated photoemission (also the inverse part) for LaSrCuO material in a wide range of doping [5]. More reliable are emission spectra related to $\mathcal{N}^+(\omega) = \mathcal{N}(\omega + \mu) f(\omega)$, giving information for $\omega < 0$. In the overdoped systems $c_h > 0.2$ $\mathcal{N}^+(\omega < 0)$ appears flat. On the other hand, for $c_h < 0.17$ a pseudogap starts to emerge gradually, e.g. the inflection point in $\mathcal{N}^+(\omega)$ moves from $\omega \sim 0$ towards $\omega \sim -0.2$eV at lowest doping. This is quite close to our results and values in Fig. 3. The pseudogap scale and its doping dependence seems thus to be related to T^* [6], appearing e.g. as the maximum in χ_0. Note however that such a gap is much larger than the leading-edge shift ~ 30meV found in ARPES [2] in underdoped samples.

In conclusion, we have shown that within the t-J model the spectral function changes with doping from that of a local FL to a strongly nonlocal one. It seems plausible that the locality of the self-energy at intermediate doping is related to the coupling of QP to large (mostly local) quantum fluctuations of the spin subsystem [16] whereby its anomalous behavior emerges due to the frustration induced by holes. The locality has several important consequences. Apart form the mentioned effect on $\mathcal{N}(\mu)$, one key feature is the reduction of FL parameters to only two, which are even simply related [14]. It is still a question whether such a local FL has properties analogous to ones obtained in infinite-D models [15].

In contrast, the nonlocality of $\Sigma(\mathbf{k}, \omega)$ induced by short-range AFM correlations becomes essential for the regime of weak doping, and is dominating the low-energy behavior $\omega \sim 0$. The most pronounced effect is the opening of the pseudogap in the DOS. $A(\mathbf{k}, \omega)$ in this regime can reveal a coexistence of a hole-like dispersion analogous to undoped AFM and an electron-like resonance. One of the challenging questions remains whether in underdoped systems we are still dealing with a well defined large FS, whereby our results do not contradict this scenario. It should also be pointed out that nonlocality is crucial to account for the marked difference in the low-doping regime between nearly free-fermion-like Wilson ratio and a strongly enhanced (possibly even singular) compressibility [11], indicating the closeness to a charge instability.

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